

homework6

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2023-04-30

Q6. How would you generalize the original code above to work with any set of input protein structures? Write your own function starting from the code above that analyzes protein drug interactions by reading in any protein PDB data and outputs a plot for the specified protein. Create a new RMarkdown document with your function code AND example output. We also suggest you include narrative text that address the rubric items below. Generate a PDF report and submit this PDF to our GradeScope site.

```
library(bio3d)
s1 <- read.pdb("4AKE") # kinase with drug

## Note: Accessing on-line PDB file

s2 <- read.pdb("1AKE") # kinase no drug

## Note: Accessing on-line PDB file
## PDB has ALT records, taking A only, rm.alt=TRUE

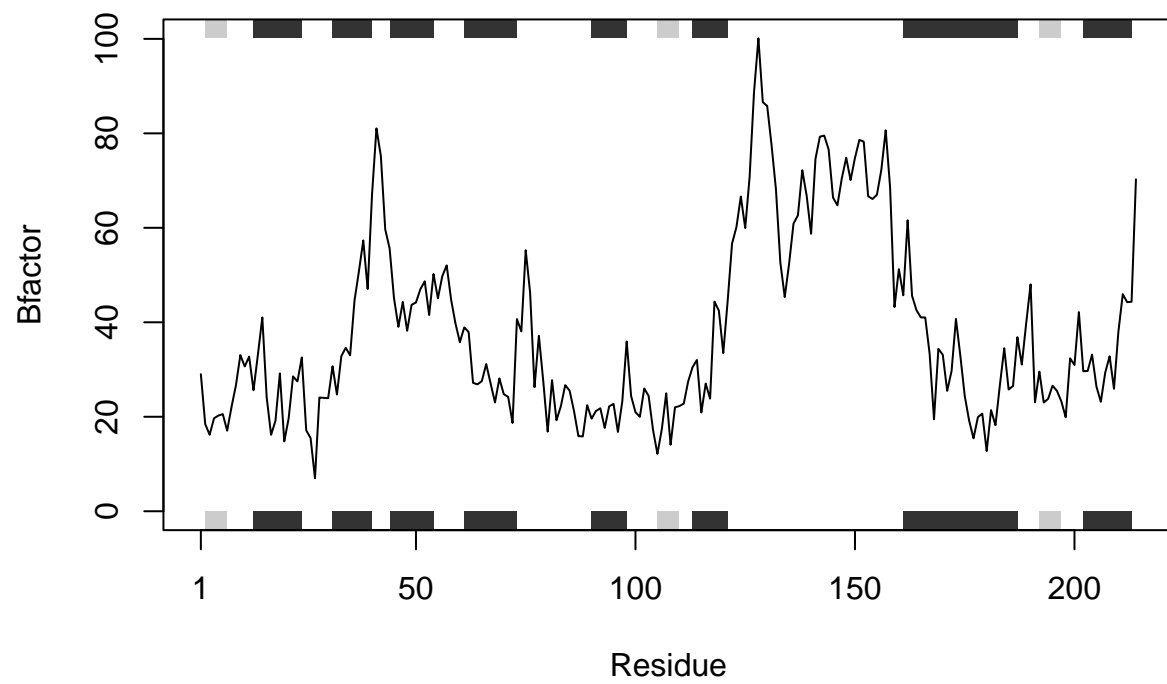
s3 <- read.pdb("1E4Y") # kinase with drug

## Note: Accessing on-line PDB file

s1.chainA <- trim.pdb(s1, chain="A", eley="CA")
s2.chainA <- trim.pdb(s2, chain="A", eley="CA")
s3.chainA <- trim.pdb(s1, chain="A", eley="CA")

s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b

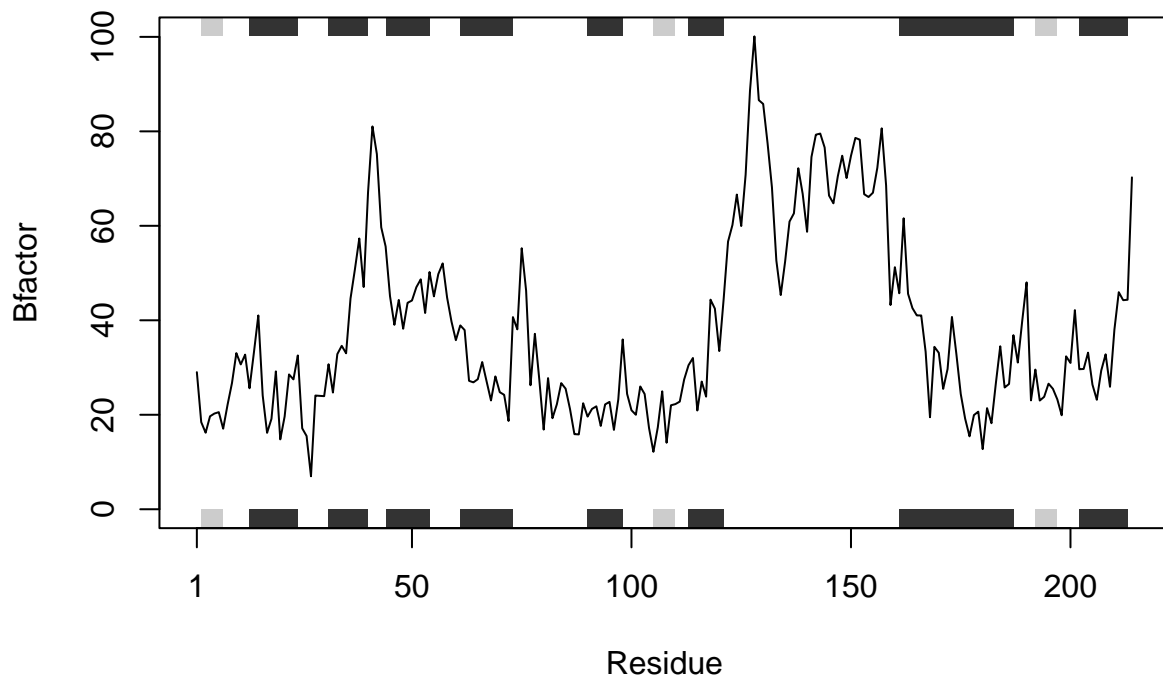
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```



```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```



Make a simple snippet

```
pdb_code <- "4AKE"
```

```
pdb <- read.pdb(pdb_code)
```

```
## Note: Accessing on-line PDB file
```

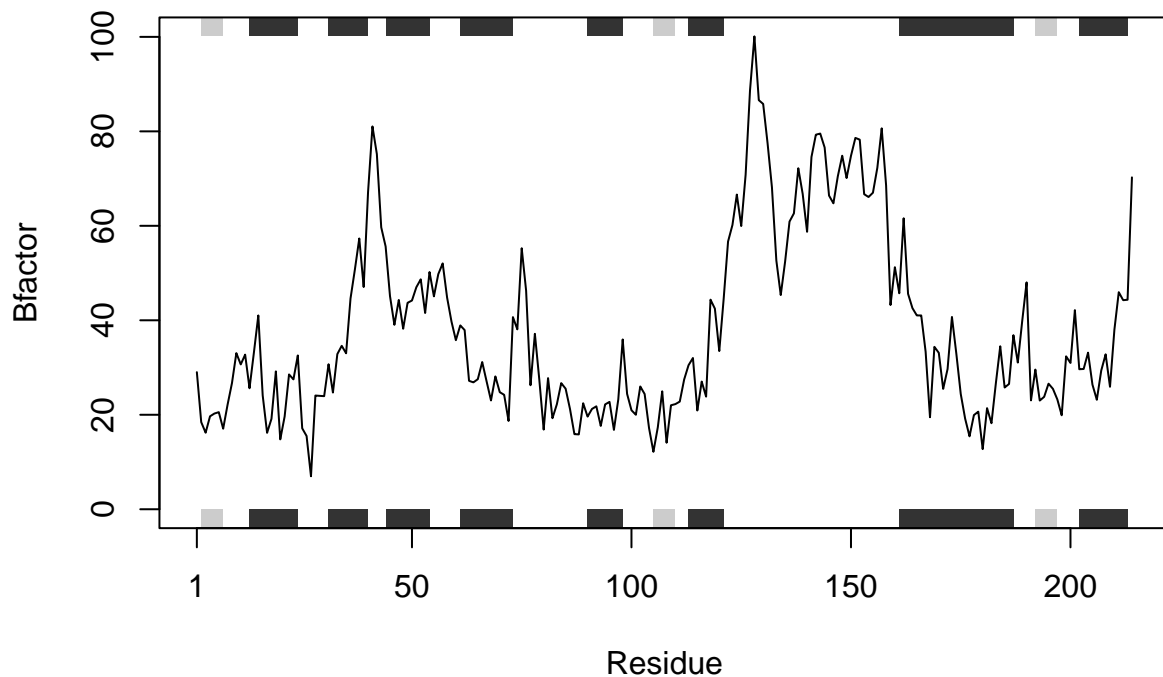
```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
```

```
## /var/folders/r2/4nybt6lx11qdr4rdnmn551jw0000gn/T//RtmpVsQcWS/4AKE.pdb exists.
```

```
## Skipping download
```

```
chain <- trim.pdb(pdb, chain="A", eley="CA")
```

```
plotb3(chain$atom$b, sse=chain, type="l", ylab="Bfactor")
```



Make a function that will allow us to plot using the pdb code.

```
analyze_pdb_code <- function(pdb_code) {
  # Read in the PDB file
  pdb <- read.pdb(pdb_code)

  # Trim the structure to only include the CA atoms of chain A
  chain <- trim.pdb(pdb, chain="A", eley="CA")

  # Extract the B-factors
  b_factors <- chain$atom$b

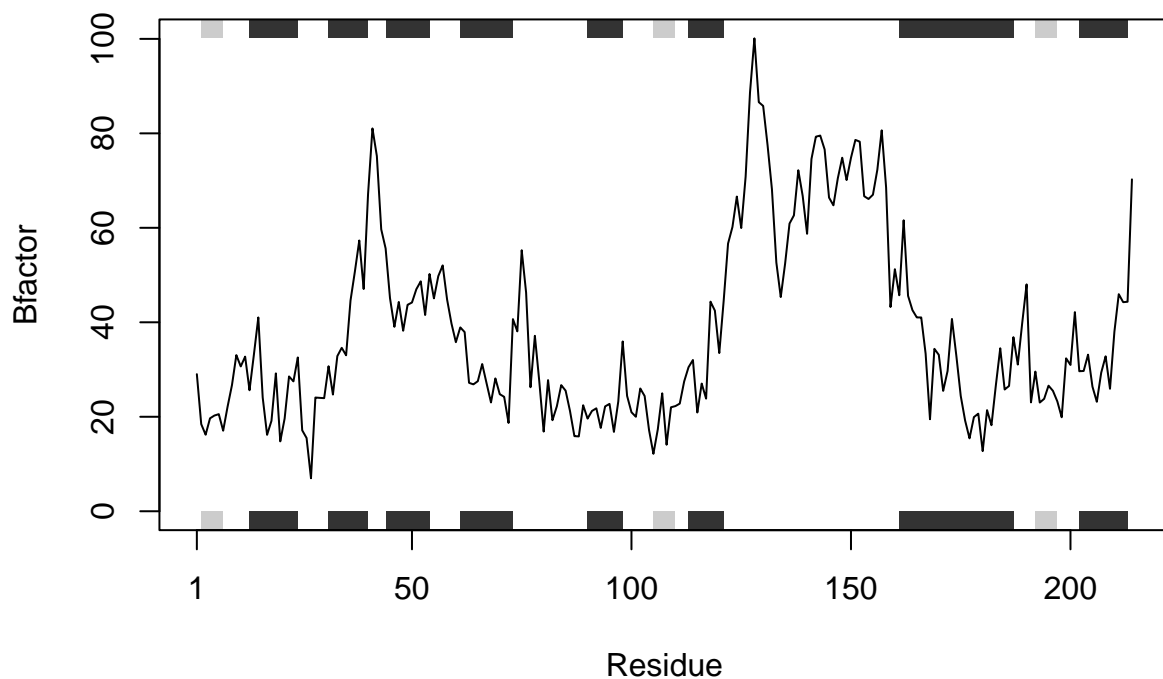
  # Plot the B-factors with secondary structure elements
  plotb3(b_factors, sse=chain, typ="l", ylab="Bfactor")
}
```

Example usage

```
analyze_pdb_code("4AKE")
```

```
## Note: Accessing on-line PDB file
```

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
## /var/folders/r2/4nybt6lx11qdr4rdnmn551jw0000gn/T//RtmpVsQcWS/4AKE.pdb exists.
## Skipping download
```



Check if the function works with the other pdb codes.

```
analyze_pdb_code("1AKE")
```

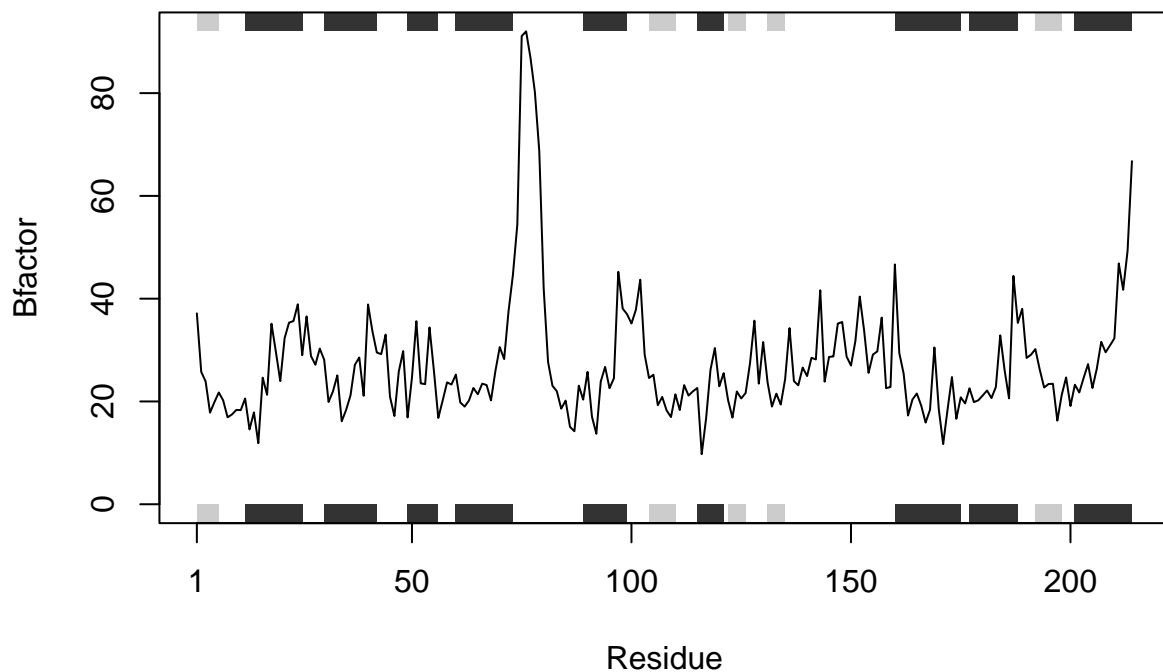
```
## Note: Accessing on-line PDB file
```

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
```

```
## /var/folders/r2/4nybt6lx11qdr4rdnmn551jw0000gn/T//RtmpVsQcWS/1AKE.pdb exists.
```

```
## Skipping download
```

```
## PDB has ALT records, taking A only, rm.alt=TRUE
```



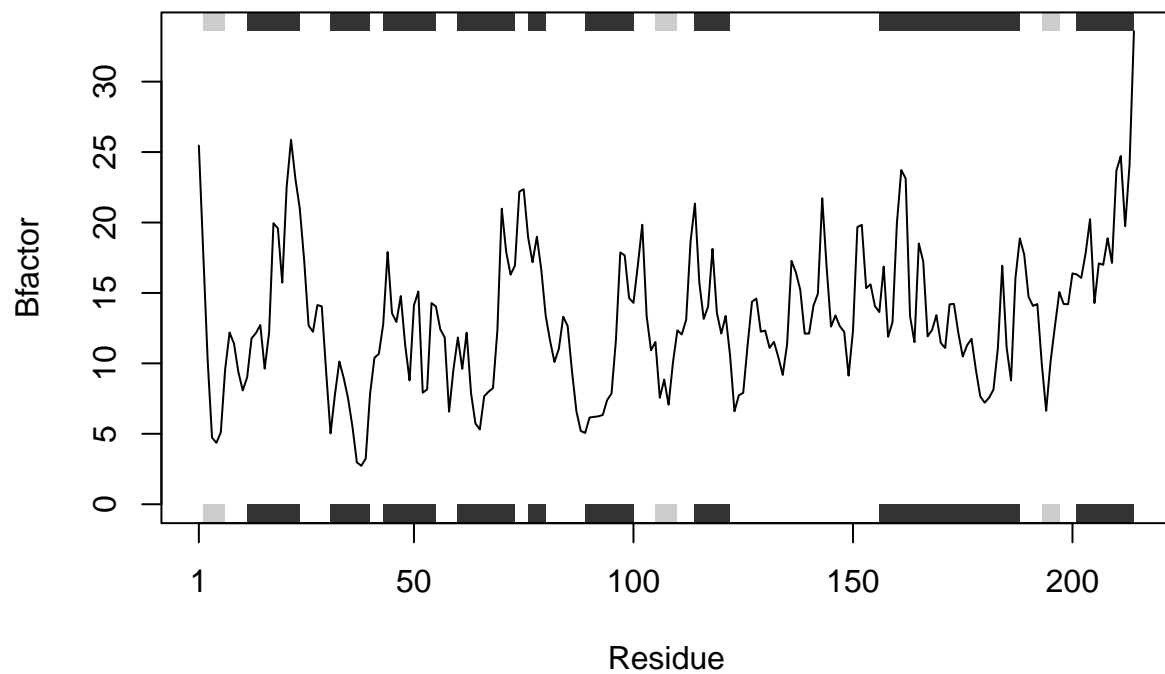
```
analyze_pdb_code("1E4Y")
```

```
## Note: Accessing on-line PDB file
```

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
```

```
## /var/folders/r2/4nybt6lx11qdr4rdnmn551jw0000gn/T//RtmpVsQcWS/1E4Y.pdb exists.
```

```
## Skipping download
```



Now we can plot using the function, avoiding mistakes.